CCP4i - "Tricks and Tools"

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CCP4i - "Tricks and Tools"

- New in CCP4i 1.3.8

- Project Management Tools
  - *Project Directories*
  - *Job Database & Project History*
  - *Electronic Notebook*
  - *Report External Tasks*

- Data Harvesting

- File Viewers
  - *Loggraph*
  - *MapSlicer*
  - *AstexViewer*

- Installing new tasks

- Preferences

New in CCP4i 1.3.8

- New interfaces:
  - OASIS
  - ACORN
  - ANISOANL, TLSANL
  - BEAST
  - PROFESSS
  - ROTAMER
  - WHAT_CHECK *(n.b. the program must currently be obtained from CMBI)*

- New CCP4i-based application GET_PROT (aka SAPHIRE)
  - *download & edit protein sequence data*

- Updated interfaces and tools:
  - SCALA
  - *Import Scaled Data task*
  - *Automatic reindexing facility in* CAD *task*
  - *Integrated viewers (*MapSlicer, AstexViewer*)*
  - *Task Interface Installer*

Project Management Tools (1)

- Why Project Management?
  - *Reminds you what you did six months ago*
  - *Helps keep track of multiple projects and associated data*
  - *Facilitates back-tracking (especially if things go wrong)*
  - *Helps when depositing results & writing your paper*

- Project Directories
  - *Set up aliases for project directories in "Project & Project Directories" Window*
  - *All data files relating to one crystallographic project should be in a single project directory*

- Job Database & Project History
  - *Stores parameters used to run each task*
  - *Records input, output and logfiles for each job*
  - *Allows you to review parameters used*
  - *Allows you to rerun a job with the same/modified parameters*

Project Management Tools (2)

Access additional tools through the "Edit Job Data" option:
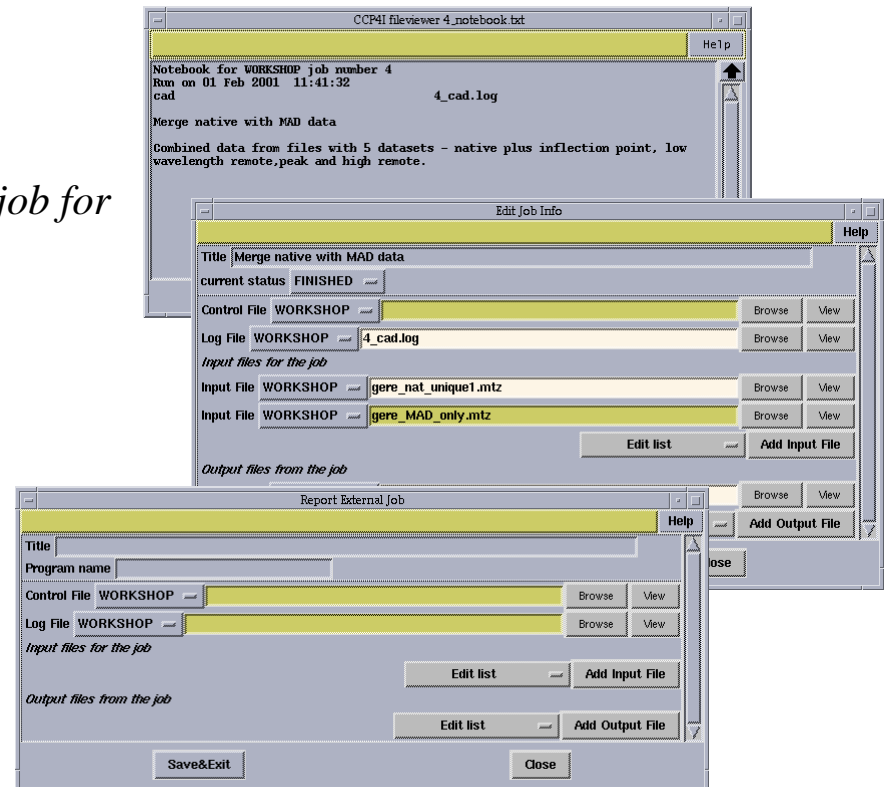

- **Electronic Notebook**
  - *Record information about a particular job for future reference*

- **Edit Job Data**
  - *Keep Job Database up-to-date*
  - *Record changes e.g. of file locations*

- **Report External Tasks**
  - *Record runs of non-CCP4(i) programs plus associated files*
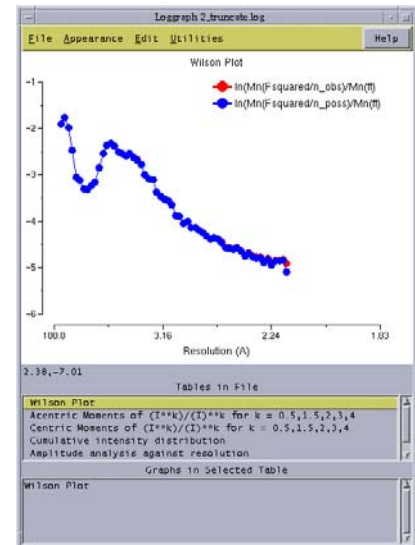 - *Keep project history complete*

Data Harvesting

- Why is it useful?
  - *Data is automatically collected in Harvest Files*
  - *The files can be deposited directly, reducing the amount of manual handling at deposition*

- What does it require?
  - *Harvesting Project & Dataset names must be defined in MTZ file*
  - *Can be done at any entry point (e.g. "import" tasks) or via "Edit Project & Dataset Name" task*

- How much work is it?
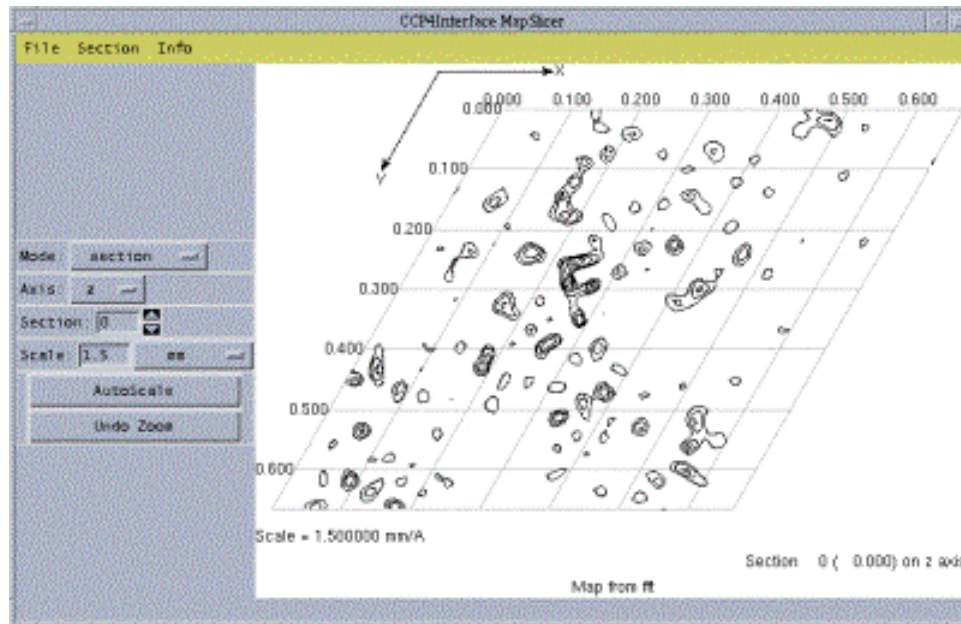 - *Switch harvesting on (or off) in Preferences or in individual tasks*
  - *That's all*

File Viewers (1)

- ## From within CCP4i:
  - ### *View Files from Job*: *always uses default file viewer*
  - ### *View Any File*: *allows you to select from available viewers*

- ## From Unix command line:
  - ### *Use* `ccp4i -v <filename>` *to view a file in the default viewer*
  - ### *Useful for MTZ files (automatically runs mtzdump program to display header)*

- ## HTML logfiles
  - ### *Can be viewed as plain text or in HTML browser*

- ## Loggraph
  - ### *View tables and graphs in CCP4-formatted logfiles*
  - ### *Can also use* `loggraph <filename>` *at the command line*
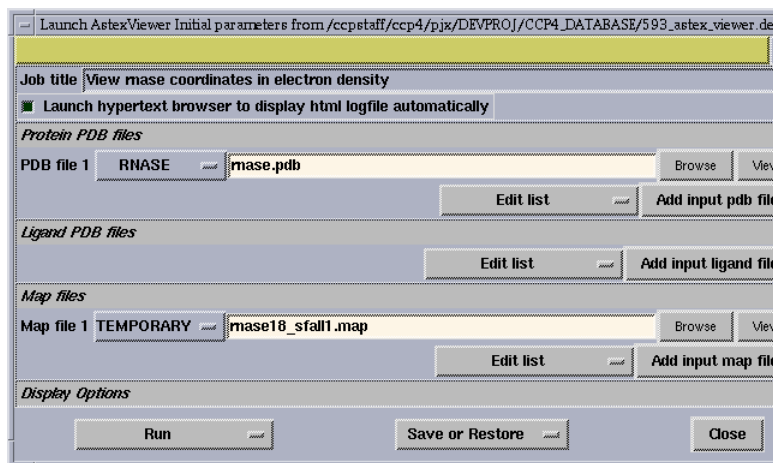
File Viewers (2)

- MapSlicer
  - *Interactive viewer for map sections*
  - *Can view single sections or slabs on x, y or z axes*
  - *Special mode for viewing Harker sections*
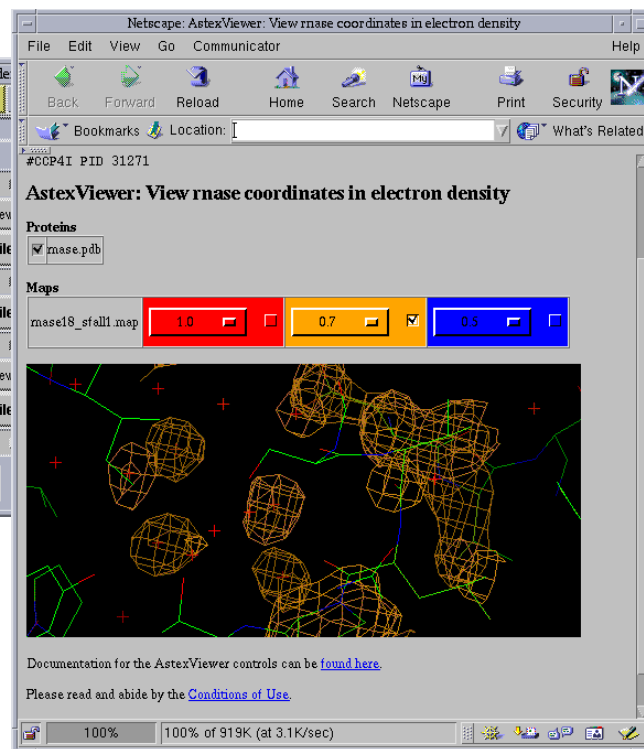 - *Can set this to be the default map viewer in "Preferences"*

File Viewers (3)

- AstexViewer
  - *Java-based protein-ligand viewer*
  - *Displays structures in electron density*
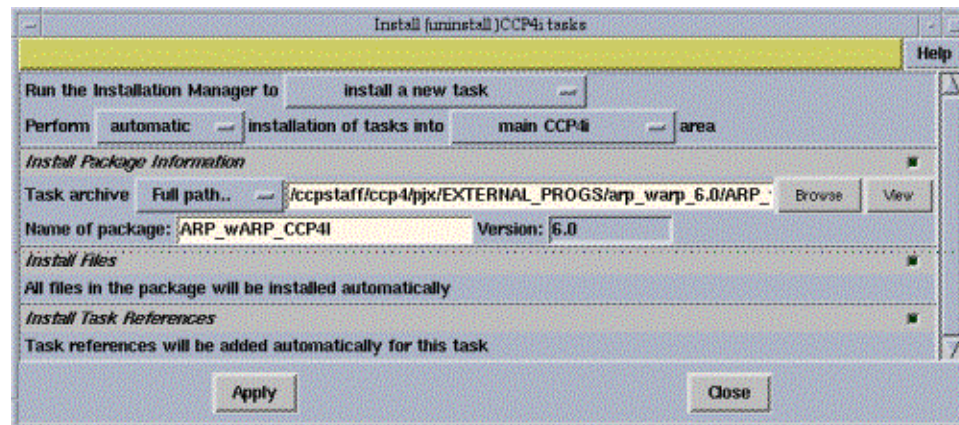 - *Can be launched from "AstexViewer" task in Program List*

- XtalView/Xfit launcher
  - *Also available for those who prefer to use XtalView - in "Model Building" module*
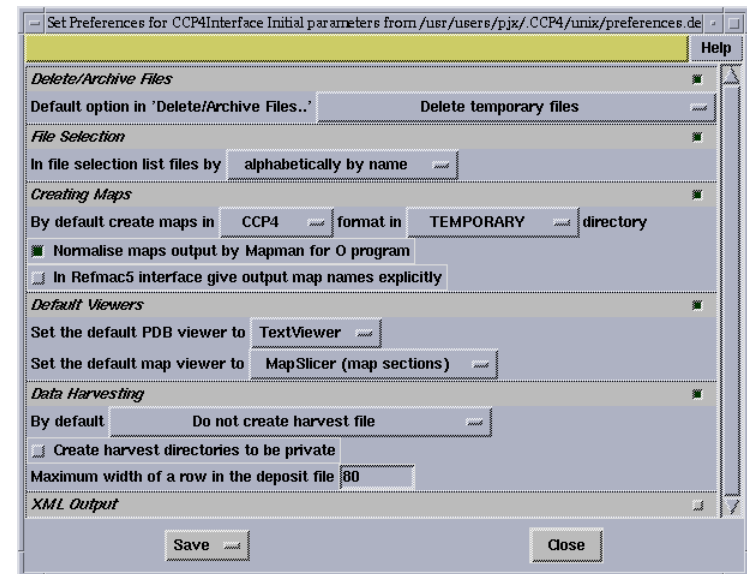
Installing New Tasks

- Install task interfaces supplied for non-CCP4i programs
  - *e.g. ARP/wARP 6.0*

- Accessed from *"System Administration"* menu
  - *New tasks installed in main CCP4i area (available to all)*
  or in user's "private" (i.e. $HOME/.CCP4/..., available only to that user)

- Allows easy review, update (and de-installation) of currently installed task interfaces

CCP4i Preferences

Set various useful things in the "Preferences":

- *Default viewers for maps & PDB files*

- *Default locations and formats for map files*

- *Default Data Harvesting mode*

Further Information …

- **Project Management Tools:**
  - *"CCP4i as a Project Management Tool" - CCP4 Newsletter 38 (April 2000)*
    `http://www.ccp4.ac.uk/newsletter38/09_projman.html`

- **MapSlicer:**
  - *"MAPSLICER: an interactive viewer for contoured map sections" - CCP4 Newsletter 39 (March 2001)*
    `http://www.ccp4.ac.uk/newsletter39/09_mapslicer.html`

- **What's New in CCP4i 1.3.8/Future Developments:**
  - *"Developments with CCP4i" - CCP4 Newsletter 41 (October 2002)*
    `http://www.ccp4.ac.uk/newsletter41/02_ccp4i-oct02/ccp4i-oct2002.html`

- **CCP4i Webpage:**
  - `http://www.ccp4.ac.uk/ccp4i_main.html`

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The End.